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# Phenomenological expressions for densities and currents in condensed media and Umklapp processes

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*Abstract.* The densities and currents of energy, momentum and quasi momentum for an elastic anisotropic continuum are discussed in terms of phonons. It is shown that these expressions are in agreement with familiar phenomenological formulae. Additionally we discuss the densities of spin and quasi angular momentum. For crystals the quasi momentum is related to the concept of Umklapp processes.

## 1. Introduction

In the companion paper [1], which we shall henceforth call I, we have studied the continuous symmetry transformations for the continuous model of the crystal. These transformations generate a set of local conservation laws or balance equations. From these equations we have found the densities of energy, momentum, quasi momentum, angular momentum, quasi angular momentum, spin, and also the current densities for these quantities. Having the expressions for currents one can find the suitable kinetic coefficients describing dissipation. For this purpose one can use the exact but formal Kubo expression. Of course, since Kubo's formula is exact the problem of calculation the analytical dependence of kinetic coefficients on the temperature, wave vector and frequency is not a trivial task and one should use some approximation schemes. In the case of transport properties of crystals one usually uses a specific basis of eigenfunctions. Namely, the basis of eigenfunctions of the harmonic part of the energy, called the phonon picture (cf. for example [2]).

On the other hand, there exist simple phenomenological theories of the transport properties of crystals in which phonons are treated as particles carrying the energy and quasi momentum [3, 4, 5, 6]. In these theories one uses definite

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expressions for the densities of energy and quasi momentum and for their currents. The form of these expressions is borrowed from the kinetic theory of rarified gases or from electrodynamics (cf. [7]).

Our expressions are microscopic and we shall compare them with phenomenological formulae, which are correct in the hydrodynamical domain. In this domain one deals with macroscopic motions, the characteristic length and time of which are several orders larger than the macroscopic length and time characterizing individual atomic motions. Hence we shall perform a suitable averaging procedure.

Having identified quasi momentum we can study the transformations generated by the total quasi momentum. We discuss them in the frame of quantum mechanics. For this purpose, following Süssmann [8], we study a simple model of a crystal, namely the linear chain.

## 2. Phonons, densities and currents

Now we shall derive expressions for densities and currents in terms of phonon variables. The purpose of doing so is twofold. Firstly, the phenomenological description of transport properties of dielectric crystals is given in terms of phonons. Thus our expressions for densities and currents can be compared with those used in phenomenological theories. Since such theories describe the hydrodynamic, i.e. macroscopic, motions in crystals, the elastic continuum approximation is well suited for such purposes. Secondly, the formula for total quasi momentum will facilitate the derivation of the quantal selection rules for the difference $\mathbf{D}=\mathbf{P}-\hat{\mathbf{P}}$. We shall study this problem in the last section.

We consider solutions of the equation of motion following from the Lagrangian given by equation I(2.1)

$$\rho_0 \ddot{u}_\mu(\mathbf{y},t)=C^{\alpha\beta}_{\mu\nu}\nabla_\alpha\nabla_\beta u_\nu(\mathbf{y},t). \tag{2.1}$$

Since this is a linear differential equation we take the solutions in the form of a Fourier decomposition

$$\begin{aligned}\mathbf{u}(\mathbf{y},t)&=V^{-1/2}\sum_{\mathbf{k}}\tilde{\mathbf{u}}(\mathbf{k},t)e^{i\mathbf{k}\cdot\mathbf{y}}\\&=V^{-1/2}\tilde{\mathbf{u}}(0,t)+V^{-1/2}\sum_{j,\mathbf{k}\neq 0}e^{i\mathbf{k}\cdot\mathbf{y}}Q_k(t)\mathbf{e}(k),\end{aligned} \tag{2.2}$$

where $V$ is the volume of the entire system and $k$ denotes the pair $(j,\mathbf{k})$. The index $j$ numerates the eigen vectors $\mathbf{e}(k)$ and eigen values $\omega^2(k)$ of the dynamical matrix $1/\rho_0 C^{\alpha\beta}_{\mu\nu}k_\alpha k_\beta$. Thus

$$1/\rho_0 C^{\alpha\beta}_{\mu\nu}k_\alpha k_\beta e_\nu(k)=\omega^2(k)e_\mu(k). \tag{2.3}$$

We may also introduce the propagation matrix $\Lambda(\hat{\mathbf{k}})$ with elements

$$\Lambda_{\mu\nu}(\hat{\mathbf{k}})=\hat{k}_\alpha\frac{1}{\rho_0}C^{\alpha\beta}_{\mu\nu}\hat{k}_\beta, \tag{2.4}$$

where $\hat{\mathbf{k}}=\mathbf{k}/|\mathbf{k}|$. Then (2.3) reads

$$\Lambda_{\mu\nu}(\hat{\mathbf{k}})e_\nu(\mathbf{k},j)=\frac{\omega^2(\mathbf{k},j)}{|\mathbf{k}|^2}e_\mu(\mathbf{k},j). \tag{2.5}$$

In cases where the propagation matrix has the two-fold degenerated eigenvalue $\lambda_1$ and the additional eigenvalue $\lambda_3$ corresponding to the eigenvector $\mathbf{e}(3)$, the propagation matrix can be written in the form of an axial propagation matrix

$$\Lambda = \lambda_1 I + (\lambda_3 - \lambda_1)\mathbf{e}(3) \times \mathbf{e}(3) \tag{2.6}$$

where $I$ is the $3\times 3$ unit matrix and the product $\mathbf{u} \times \mathbf{v}$ means

$$(\mathbf{u} \times \mathbf{v})_{\mu\nu} = u_\mu v_\nu. \tag{2.7}$$

In case of a 3-fold degenerated eigenvalue $\lambda$, the propagation matrix $\Lambda$ is the so called isotropic propagation matrix

$$\Lambda = \lambda \sum_{i=1}^{3} \mathbf{e}(i) \times \mathbf{e}(i) = \lambda I. \tag{2.8}$$

Let us choose the normal coordinates $Q_k$ in the form of the combination of phonon variables $a_k$ and $a_k^*$ ($\mathbf{k} \neq 0$, $-k = (j, -\mathbf{k})$)

$$Q_k = \sqrt{\frac{\hbar}{2\rho_0 \omega(k)}} A_k; \qquad A_k = a_k + a_{-k}^* \tag{2.9}$$

Similarly, for the linear momentum we set

$$\begin{aligned}\mathbf{p}(\mathbf{y}, t) &= V^{-1/2} \sum_{\mathbf{k}} \tilde{\mathbf{p}}(\mathbf{k}, t) e^{-i\mathbf{k}\cdot\mathbf{y}} \\ &= V^{-1/2}\tilde{\mathbf{p}}(0, t) + V^{-1/2} \sum_{j,\mathbf{k}\neq 0} \frac{1}{i} \sqrt{\frac{\hbar \rho_0 \omega(k)}{2}}\, e^{-i\mathbf{k}\cdot\mathbf{y}} \mathbf{e}(-k) B_k \end{aligned} \tag{2.10}$$

where

$$B_k = a_{-k} - a_k^*.$$

Then the Hamiltonian constructed from the Lagrangian I (2.1) takes the general form

$$H = \frac{1}{2\rho_0 V} \tilde{\mathbf{p}}(0, t) \cdot \tilde{\mathbf{p}}(0, t) + \sum_{j,\mathbf{k}\neq 0} \hbar\omega(k)(a_k^* a_k + a_k a_k^*). \tag{2.11}$$

It is an easy task to show that the zero Fourier harmonic $\tilde{\mathbf{p}}(0, t)$ is proportional to the lattice momentum. Indeed tracing back from the field $\tilde{\mathbf{p}}(\mathbf{k}, t)$ to the corresponding lattice variable, one finds

$$\begin{aligned}\tilde{\mathbf{p}}(0, t) &= V^{-1/2} \int d^3y\, \mathbf{p}(\mathbf{y}) e^{-i\mathbf{k}\cdot\mathbf{y}} \Big|_{\mathbf{k}=0} \\ &= V^{-1/2} \int \mathbf{p}(\mathbf{y})\, d^3y = V^{-1/2}\mathbf{P} = V^{1/2}\langle \mathbf{p} \rangle \end{aligned} \tag{2.12}$$

where $\mathbf{P}$ is the total linear momentum and $\langle \mathbf{p} \rangle$ the linear momentum per unit of volume. Similarly one finds

$$\begin{aligned}\tilde{\mathbf{u}}(0, t) &= V^{-1/2} \int d^3y\, \mathbf{u}(\mathbf{y}) e^{i\mathbf{k}\cdot\mathbf{y}} \Big|_{\mathbf{k}=0} = V^{-1/2} \int \mathbf{u}(\mathbf{y})\, d^3y \\ &= V^{-1/2} \langle \mathbf{u} \rangle, \end{aligned} \tag{2.13}$$

$\langle \mathbf{u} \rangle$ being the average displacement of one atom.

The first term of the Hamiltonian (2.11) now is simply the kinetic energy of the center of mass

$$\frac{1}{2M}\mathbf{P}^2=\tfrac{1}{2}M\dot{\mathbf{R}}^2, \tag{2.14}$$

where $M=\rho_0 V$ is the total mass of the system and $\dot{\mathbf{R}}=\mathbf{P}/M$ is the velocity of the center of mass.

As we see, the state of a crystal is described in terms of the center of mass variables and the phonon variables. In the quantum case these two sets of variables mutually commute. They belong to different Fourier harmonics.

Next we shall quantize the canonically conjugated fields $\mathbf{u}$, $\mathbf{p}$. We impose the condition of the canonical commutation rule

$$[u_\alpha(\mathbf{y}), p_\beta(\mathbf{y}')]=i\hbar\delta_{\alpha,\beta}\delta(\mathbf{y}-\mathbf{y}'). \tag{2.15}$$

For the Fourier transforms we get from the above commutation rule

$$[\tilde{u}_\alpha(\mathbf{k}), \tilde{p}_\beta(\mathbf{k}')]=i\hbar\delta_{\alpha,\beta}\delta_{\mathbf{k},\mathbf{k}'}, \tag{2.16}$$

and the center of mass variables obey the commutation rule

$$[R_\mu, P_\nu]=i\hbar\delta_{\mu\nu}, \tag{2.17}$$

whereas these commute with the other harmonics $p_\mu(\mathbf{k})$ and $u_\nu(\mathbf{k})$. The phonon operators obey the Bose communication rules

$$[a_k, a^*_{k'}]=\delta_{k,k'}=\delta_{\mathbf{k},\mathbf{k}'}\delta_{j,j'} \tag{2.18}$$

and additionally

$$[a_k, \mathbf{R}]=[a^*_k, \mathbf{R}]=[a_k, \mathbf{P}]=[a^*_k, \mathbf{P}]=0. \tag{2.19}$$

With the use of these commutation rules the Hamiltonian takes the familiar form

$$H=\frac{1}{2M}\mathbf{P}^2+\sum_{j,k\neq 0}\hbar\omega(k)(a^*_k a_k+\tfrac{1}{2}). \tag{2.20}$$

The time dependent classical fields should be understood now as quantum fields in the Heisenberg picture. This means that the phonon variables oscillate, e.g.

$$a_k(t)=e^{-i\omega(k)t}a_k; \qquad a^*_k(t)=e^{-i\omega(k)t}a^*_k. \tag{2.21}$$

As a consequence the densities and current densities oscillate in time and in space. Often in macroscopic experiments, these oscillations are difficult to detect and not of interest. For this reason we shall average these quantities. We define the averaged smooth quantities with the help of space integrals, e.g.

$$\langle\mathbf{p}(\mathbf{y})\rangle=\frac{1}{V}\int d^3y\,\mathbf{p}(\mathbf{y})=\frac{1}{V}\mathbf{P}, \tag{2.22}$$

the total linear momentum per unit of volume. The smoothed energy density is the total energy per unit volume and contains two parts

$$\langle e(\mathbf{y})\rangle=\frac{1}{V}\left(\frac{1}{2M}\mathbf{P}^2+\sum_{j,k\neq 0}\hbar\omega(k)(a^*_k a_k+\tfrac{1}{2})\right). \tag{2.23}$$

For the smoothed quasi-momentum density one obtains similarly

$$\langle\hat{\mathbf{P}}(\mathbf{y})\rangle=\frac{1}{V}\sum_{j,k\neq 0}\hbar\mathbf{k}a_k^*a_k \tag{2.24}$$

and the average of the current density of momentum vanishes

$$\langle\pi_{\beta\nu}(\mathbf{y})\rangle=0. \tag{2.25}$$

The averages of the current densities for energy and quasi momentum are more complicated. After some straightforward calculations (e.g. see [1, 10]) one finds

$$\begin{aligned}\langle j_\alpha^E\rangle&=\frac{1}{V}\sum_{j,k\neq 0}\hbar\omega(k)\frac{\partial\omega(k)}{\partial k_\alpha}a_k^*a_k\\&+\frac{\hbar}{4V}\sum_{j,j',k\neq 0}\left(\frac{\omega(k,j)}{\omega(k,j')}\right)^{1/2}(\omega^2(\mathbf{k},j)-\omega^2(\mathbf{k},j'))\\&\times e_\mu^*(\mathbf{k},j)\frac{\partial e_\mu(\mathbf{k},j)}{\partial k_\alpha}(A_{\mathbf{k},j}B_{-\mathbf{k},j'}+B_{-\mathbf{k},j'}A_{\mathbf{k},j}).\end{aligned} \tag{2.26}$$

In the Heisenberg picture, the operator part of the non-diagonal term of $j_\alpha^E$ oscillates rapidly. Hence, the time average, which we denote with a bar, gives

$$\begin{aligned}\overline{\langle j_\alpha^E(\mathbf{y},t)\rangle}&=\lim_{T\to\infty}\frac{1}{T}\int_0^T dt\langle j_\alpha^E(y,t)\rangle\\&=\frac{1}{V}\sum_{j,\mathbf{k}\neq 0}\hbar\omega(k)\frac{\partial\omega(k)}{\partial k_\alpha}a_k^*a_k\end{aligned} \tag{2.27}$$

This formula shows that the energy is transported with the group velocity $\mathbf{v}(k)=(\partial/\partial\mathbf{k})\omega(k)$, as is generally assumed in phenomenological theories.

As we have checked the space average of $\pi_{\alpha\mu}(\mathbf{y},t)$ vanishes. This is in agreement with the transport theory, since it is well known that not the momentum but the quasi momentum plays an essential role in transport theory [3, 4]. Thus beside the arguments about the importance of quasi momentum non-conserving processes for reducing the heat conductivity to a finite value [3, 4], we see that our expressions for the operators of densities show that the proper momentum cannot play an important role in the heat transport of crystals (cf. also Section 5). This is also in agreement with the physical argumentation. In specimen with a temperature gradient, the phonons are created, but the crystal does not move. Thus only the quasi momentum is changing.

Finally we obtain the formula for the space and time average of the current density for quasi momentum [10], also in agreement with the phenomenological theories [3, 6]

$$\overline{\langle\hat{\pi}_{\alpha\gamma}(\mathbf{y},t)\rangle}=\frac{1}{V}\sum_{j,k\neq 0}\hbar k_\alpha\frac{\partial\omega(k)}{\partial k_\gamma}a_k^*a_k \tag{2.28}$$

In closing this section it is worthwhile to underline that we have got quite strong results for momentum and quasi-momentum density. The formulae (2.17) and (2.19) do not depend on the approximations made in the model (continuous harmonic approximation). All other results do depend on these assumptions. So the smoothed linear momentum flux density $\langle \pi_{\mu\nu}(\mathbf{y}) \rangle$ will generally not vanish but depends on the non-harmonic terms in the Hamiltonian. This is of importance e.g. for the explanation of sound pressure [11]. The expressions found for the smoothed energy (current) density and quasi momentum (current) density hold as far as the harmonic approximation is allowed. But their form does not depend on the approximations we have used [2, 10].

## 3. Spin and (quasi) angular momentum density

In I we have derived the (approximative) global conservation laws for proper angular momentum

$$d_t \int d^3y (S_\rho(\mathbf{y}) + L_\rho(\mathbf{y})) \doteq \int \mathscr{E}_{\nu\rho\lambda} \pi_{\beta\nu} \nabla_\beta u_\nu \, d^3y \approx 0 \tag{3.1}$$

and for the quasi angular momentum

$$d_t \int d^3y (S_\rho(\mathbf{y}) + \hat{L}_\rho(\mathbf{y})) \doteq \int \mathscr{E}_{\nu\rho\lambda} \pi_{\beta\nu} (\nabla_\beta u_\nu + \nabla_\nu u_\beta) \, d^3y \approx 0 \tag{3.2}$$

valid for $|\nabla u| \ll 1$.

In this section we will investigate the smoothed densities of the proper and of the quasi angular momentum in terms of phonon variables. Let us first look at the orbital part $L_\rho(\mathbf{y})$ of the proper angular momentum

$$L_\rho(\mathbf{y}) = \rho_0 \mathscr{E}_{\rho\mu\nu} y_\mu \dot{u}_\nu. \tag{3.3}$$

With (2.10) and suitable boundary conditions one easily finds

$$\langle \mathbf{L}(\mathbf{y}) \rangle = \frac{1}{V} \int d^3y \mathbf{L}(\mathbf{y}) = \frac{1}{V} \int d^3y \mathbf{y} \wedge \mathbf{P}. \tag{3.4}$$

So, only the motion of the center of mass contributes to the orbital part of the averaged angular momentum.

Consider now the orbital part of the quasi angular momentum

$$\hat{L}_\rho(y) = -\rho_0 \mathscr{E}_{\gamma\rho\lambda} y_\lambda \dot{u}_\mu \nabla_\gamma u_\mu. \tag{3.5}$$

With (2.2) and (2.5) one finds

$$\begin{aligned}\langle \hat{L}_\rho \rangle &= \frac{1}{V} \int d^3y L_\rho(\mathbf{y}) = -\frac{1}{V} \mathscr{E}_{\rho\mu\nu} \int d^3y y_\mu p_\alpha \nabla_\nu u_\alpha \\ &= \frac{-i}{V^2} \mathscr{E}_{\rho\mu\nu} \int d^3y y_\mu \tilde{p}_\alpha(0) \sum_{\mathbf{k}'\neq 0} k'_\nu \tilde{u}_\alpha(\mathbf{k}') e^{i\mathbf{k}'\cdot\mathbf{y}} \\ &\quad \frac{-i}{V^2} \mathscr{E}_{\rho\mu\nu} \int d^3y \sum_{\mathbf{k},\mathbf{k}'\neq 0} y_\mu k'_\nu \tilde{p}_\alpha(\mathbf{k}) \tilde{u}_\alpha(\mathbf{k}') e^{-i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{y}}.\end{aligned} \tag{3.6}$$

For usual macroscopic systems, the allowed values of $\mathbf{k}$ are distributed almost continuously. Therefore the summations over $\mathbf{k}$ and $\mathbf{k}'$ may be approximated by integrals

$$\sum_{\mathbf{k}} \to \frac{V}{(2\pi)^3} \int d^3k. \tag{3.7}$$

In this way we find

$$\begin{aligned}\langle \hat{L}_\rho \rangle = & -\frac{1}{V^2} \frac{V}{(2\pi)^3} \mathscr{E}_{\rho\mu\nu} \tilde{p}_\alpha(0) \int d^3k' k'_\nu \tilde{u}_\alpha(\mathbf{k}') \frac{\partial}{\partial k'_\mu} \int d^3y e^{i\mathbf{k}'\cdot\mathbf{y}} \\ & + \frac{1}{V^2} \frac{V^2}{(2\pi)^6} \mathscr{E}_{\rho\mu\nu} \int d^3k \int d^3k' k'_\nu \tilde{p}_\alpha(\mathbf{k}) \tilde{u}_\alpha(k') \frac{\partial}{\partial k_\mu} \int d^3y e^{-i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{y}},\end{aligned} \tag{3.8}$$

from which easily follows

$$\langle \hat{L}_\rho \rangle = \frac{-1}{(2\pi)^3} \mathscr{E}_{\rho\mu\nu} \int d^3k k_\nu \left( \frac{\partial}{\partial k_\mu} \tilde{p}_\alpha(\mathbf{k}) \right) \tilde{u}_\alpha(\mathbf{k}). \tag{3.9}$$

We will not investigate this relation any further.

For the volume average of the intrinsic (quasi) angular momentum (= spin) $\langle \mathbf{S} \rangle$ one finds

$$\langle \mathbf{S} \rangle = \langle \mathbf{S}^0 \rangle + \langle \mathbf{S}^1 \rangle, \tag{3.10}$$

where

$$\langle \mathbf{S}^0 \rangle = \langle \mathbf{u} \rangle \wedge \langle \mathbf{p} \rangle \tag{3.11}$$

and

$$\begin{aligned}\langle \mathbf{S}^1 \rangle &= \frac{1}{V^2} \int d^3y \sum_{k,k'=0} \tilde{\mathbf{u}}(\mathbf{k}) \wedge \tilde{\mathbf{p}}(\mathbf{k}') e^{i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{y}} \\ &= \frac{\hbar}{2iV} \sum_{\mathbf{k},j,j'} \sqrt{\frac{\omega(k, j')}{\omega(k, j)}} (a_{k,j} + a^*_{-k,j})(a_{-k,j'} - a^*_{k,j'}) \\ &\quad \times \mathbf{e}(\mathbf{k}, j) \wedge \mathbf{e}^*(\mathbf{k}, j')\end{aligned} \tag{3.12}$$

Neglecting rapidly oscillating terms, one finds

$$\overline{\langle \mathbf{S}^1 \rangle} = \frac{\hbar}{2V} \sqrt{\frac{\omega(k, j')}{\omega(k, j)}} \sum_{\mathbf{k},j,j'} (\overline{i a_{\mathbf{k},j} a^*_{\mathbf{k},j'}} \mathbf{e}(\mathbf{k}, j) \wedge \mathbf{e}^*(\mathbf{k}, j') + \text{h.c.}),$$

where h.c. stands for the Hermitean conjugate.

Also the term $a_{k,j} a^*_{k,j'}$ is rapidly oscillating, unless $\omega(\mathbf{k}, j) = \omega(\mathbf{k}, j')$. Thus

$$\langle \mathbf{S}^1 \rangle = \frac{\hbar}{2V} \sum_{\mathbf{k},j,j'} (i a_{\mathbf{k},j} a^*_{\mathbf{k},j'} e(\mathbf{k}, j) \wedge e^*(\mathbf{k}, j') + \text{h.c.}), \tag{3.13}$$

where the summation has to be carried out over all degenerated states $(\mathbf{k}, j)$ and $(\mathbf{k}, j')$. Thus, in the general case where there is no degeneration, the smoothed spin density $\overline{\langle \mathbf{S}^1 \rangle}$ is identical to zero. The smoothed spin density will not vanish if there is some degeneration. This may be the case for waves propagating along symmetry axes of the medium, but it also might be the case for waves propagating in other (accidental) directions if special relations among the elements of the propagation matrix are fulfilled (cf. Federov [12]).

## 4. The smoothed spin density in case of degeneration

In this section we want to investigate the expression (3.14)

$$\langle\overline{\mathbf{S}^1}\rangle = \frac{\hbar}{2V}\sum_{\mathbf{k},j,j'}(ia_{\mathbf{k},j}a^*_{\mathbf{k},j'}\mathbf{e}(\mathbf{k},j)\wedge\mathbf{e}^*(\mathbf{k},j') + \text{h.c.}) \tag{4.1}$$

where the summation is done over all degenerated energy levels $\omega(\mathbf{k},j) = \omega(\mathbf{k},j')$.

As the polarization vectors $\mathbf{e}(\mathbf{k},j)$ are the eigen vectors of a real symmetric matrix, they can be chosen real and orthonormal:

$$\begin{aligned} &\mathbf{e}(\mathbf{k},1)\wedge\mathbf{e}(\mathbf{k},2) = \mathbf{e}(\mathbf{k},3) \quad \text{(cycl.)} \\ &\mathbf{e}(\mathbf{k},j)\cdot\mathbf{e}(\mathbf{k},j') = \delta_{j,j'} \qquad (j,j' = 1,2,3), \\ &\mathbf{e}(\mathbf{k},j) = \mathbf{e}^*(\mathbf{k},j) \qquad (j = 1,2,3). \end{aligned} \tag{4.2}$$

Assuming the energy levels numbered 1 and 2 are degenerated, any linear combination of $\mathbf{e}(\mathbf{k},1)$ and $\mathbf{e}(\mathbf{k},2)$ is again an eigen vector. Thus instead of $\mathbf{e}(\mathbf{k},j)$ $(j = 1,2,3)$ we may introduce the new base

$$\begin{aligned} &\mathbf{e}_+ = \frac{1}{\sqrt{2}}(\mathbf{e}(\mathbf{k},1) + i\mathbf{e}(\mathbf{k},2)), \\ &\mathbf{e}_- = \mathbf{e}_+^* = \frac{1}{\sqrt{2}}(\mathbf{e}(\mathbf{k},1) - \mathbf{i}\mathbf{e}(\mathbf{k},2)) \\ &\mathbf{e}_3 = \mathbf{e}(\mathbf{k},3). \end{aligned} \tag{4.3}$$

One now easily verifies

$$\begin{aligned} &\mathbf{e}_+\cdot\mathbf{e}_-^* = \mathbf{e}_-\cdot\mathbf{e}_+^* = \mathbf{e}_+\cdot\mathbf{e}_+ = \mathbf{e}_-\cdot\mathbf{e}_- = 0, \\ &\mathbf{e}_+\cdot\mathbf{e}_+^* = \mathbf{e}_-\cdot\mathbf{e}_-^* = \mathbf{e}_+\cdot\mathbf{e}_- = \mathbf{e}_-\cdot\mathbf{e}_+ = 1 \\ &\mathbf{e}_+\cdot\mathbf{e}_3 = \mathbf{e}_-\cdot\mathbf{e}_3 = 0. \end{aligned} \tag{4.4}$$

Furthermore

$$\begin{aligned} &\mathbf{e}_+\wedge\mathbf{e}_+^* = -\mathbf{e}_-\wedge\mathbf{e}_-^* = -i\mathbf{e}_3, \ \mathbf{e}_3\wedge\mathbf{e}_3^* = 0, \\ &\mathbf{e}_-\wedge\mathbf{e}_+^* = \mathbf{e}_+\wedge\mathbf{e}_-^* = 0. \\ &\mathbf{e}_3\wedge\mathbf{e}_-^* = -\mathbf{e}_+\wedge\mathbf{e}_3^* = -i\mathbf{e}_+ \\ &\mathbf{e}_3\wedge\mathbf{e}_+^* = -\mathbf{e}_-\wedge\mathbf{e}_3^* = i\mathbf{e}_- \end{aligned} \tag{4.5}$$

Now let $\omega(\mathbf{k},1) = \omega(\mathbf{k},2) \neq \omega(\mathbf{k},3)$, then with the base vectors $\mathbf{e}_+$, $\mathbf{e}_-$ and $\mathbf{e}_3$, equation (4.1) reads

$$\langle\overline{S^1}\rangle = \sum_k \hbar(-N_{\mathbf{k}+} + N_{\mathbf{k}-})\mathbf{e}_3 \tag{4.6}$$

where

$$N_{\mathbf{k}\pm} = \frac{1}{2V}(a_{\mathbf{k}\pm}a^*_{\mathbf{k}\pm} + \text{h.c.}) \tag{4.7}$$

represents the number of phonons per unit of volume with polarization $\pm$. Thus each phonon with polarization $\pm$ gives a contribution $\mp\hbar$ to the smoothed spin density in the $\mathbf{e}_3$ direction. The smoothed spin density in the other directions vanishes. In the special case of the isotropic elastic medium, for any direction of $\mathbf{k}$, the propagation matrix is axial

$$\Lambda(\hat{\mathbf{k}})=\frac{a}{\rho_0}I+\frac{a+c}{\rho_0}\hat{\mathbf{k}}\times\hat{\mathbf{k}}.$$

Then in the above formulae, the $\mathbf{e}_3$ direction equals the $\mathbf{k}$ direction and equation (4.6) reads

$$\langle\overline{S^1}\rangle=\hbar(N_{\mathbf{k}-}-N_{\mathbf{k}+})\frac{\mathbf{k}}{|\mathbf{k}|}. \tag{4.8}$$

and $N_{k+}$ and $N_{k-}$ correspond to the number of right- and left- circular polarized transversal phonons, respectively. In their study of the homogeneous isotropic elastic medium, Vonsovskii and Svirskii [9] obtain a similar result. The authors formulate this result by saying, transversal phonons have spin 1, longitudinal phonons do not carry any spin. We further refer to Levine [13] and to Jensen and Nielsen [14].

In the case of an isotropic propagation matrix $\Lambda(\hat{\mathbf{k}})=a/\rho_0\ I$ all three eigenvalues are degenerated and equal to $a/\rho_0$:

$$\omega^2(\mathbf{k},1)=\omega^2(\mathbf{k},2)=\omega^2(\mathbf{k},3)=\frac{a}{\rho_0}k^2$$

This situation corresponds to $I$ (2.3) with $c=a$. The equation of motion then is

$$\rho_0\ddot{u}=a\Delta u.$$

Choosing $\mathbf{e}_3=\mathbf{k}/|\mathbf{k}|$, as before we can define the base $\mathbf{e}_+$, $\mathbf{e}_-$, $\mathbf{e}_3$ and one obtains

$$\langle\overline{S^1}\rangle=\hbar\sum_k(-N_{\mathbf{k}+}+N_{\mathbf{k}-})\mathbf{e}_3+\langle\overline{S^1}\rangle_{\text{nd}},$$

where

$$\langle\overline{S^1}\rangle_{\text{nd}}=\frac{\hbar}{V}\sum_{\mathbf{k}}((a_3a_-^*-a_+a_3^*)\mathbf{e}_++(a_-a_3^*-a_3a_+^*)\mathbf{e}_-)$$

or

$$\langle\overline{S^1}\rangle_{\text{nd}}=\frac{\hbar}{V}\sum_{\mathbf{k}}\frac{1}{\sqrt{2}}((a_3a_-^*-a_+a_3^*+\text{h.c.})\mathbf{e}(\mathbf{k},1)$$
$$+(ia_3a_-^*-ia_+a_3^*+\text{h.c.})\mathbf{e}(\mathbf{k},2))$$

Thus, as before, with respect to the smoothed spin density in the $\mathbf{k}$ direction, circular polarized phonons behave as quasi particles with spin 1. The longitudinal polarized phonons now contribute to the smoothed spin density in a direction perpendicular to $\mathbf{k}$.

## 5. The selection rule for the quasi momentum

In the case of a crystal, an arbitrary space shift of the coordinate frame is not an exact symmetry operation. The reason lies in the discrete structure of the crystal. Let us consider the discrete operation generated by the difference operator $D = \hat{P} - P$. For a linear mono-atomic chain with interatomic distance $a$ Süssmann [8] has shown that the operator

$$\mathcal{P}_{na} = e^{iDna/\hbar} \tag{5.1}$$

generates the cyclic permutation

$$\mathcal{P}_{na} R_l \mathcal{P}_{-na} = R_{l-na}, \qquad \mathcal{P}_{na} P_l \mathcal{P}_{-na} = P_{l-na}$$
$$(n, l = 0, 1, 2, \ldots, N), \tag{5.2}$$

which does not change the variables of the center of mass

$$\mathcal{P}_{na} R \mathcal{P}_{-na} = R, \qquad \mathcal{P}_{na} P \mathcal{P}_{-na} = P. \tag{5.3}$$

The proof relies essentially on the cyclic boundary conditions. The cyclic permulation does not change the Hamiltonian

$$\mathcal{P}_{na} H \mathcal{P}_{-na} = H \; (n = 0, \pm 1, \ldots .). \tag{5.4}$$

From this invariance property the selection rule for the quasi momentum easily follows. To show this we first introduce the eigen states

$$|\sigma\rangle = |P, \ldots, n_k \ldots \ldots\rangle$$

of the harmonic part of the Hamiltonian (2.15), of $P$ and $\hat{P}$ simultaneously. The corresponding eigenvalues are $E_\sigma = \sum \frac{1}{2}\hbar\omega(k)(n_k + \frac{1}{2})$, $P_\sigma = P$ and $\hat{P}_\sigma = \sum \hbar k n_k$, respectively. Then

$$e^{inaD/\hbar} |\sigma\rangle = e^{inaD_\sigma/\hbar}; \qquad D_\sigma = \hat{P}_\sigma - P_\sigma. \tag{5.5}$$

From (5.5) and the fact that $\mathcal{P}_{na}$ commutes with the harmonic part of the Hamiltonian, now follows

$$\langle\sigma| H_{anh} |\sigma'\rangle (e^{inaD_\sigma/\hbar} - e^{inaD_{\sigma'}/\hbar}) = 0, \tag{5.6}$$

where $H_{anh}$ is the anharmonic part of the Hamiltonian, describing the interaction of the phonons. Hence, the transition probability $|\langle\sigma |H_{anh}| \sigma'\rangle|^2$ from the state $|\sigma\rangle$ into the state $|\sigma'\rangle$ is zero unless

$$e^{inaD_\sigma/\hbar} - e^{inaD_{\sigma'}/\hbar} = 0. \tag{5.7}$$

Hence the transition $|\sigma\rangle \to |\sigma'\rangle$ is possible if and only if equation (5.7) is satisfied, i.e. if the difference $(D_\sigma - D_{\sigma'})/\hbar$ equals a vector of the reciprocal lattice $G_n = 2\pi n/a$

$$D_\sigma - D_{\sigma'} = 2\pi n/a, \qquad n = 0, \pm 1, \pm 2, \ldots . \tag{5.8}$$

Thus the difference $D$ of momentum and quasi momentum is conserved only if in (5.8) $n = 0$. These processes are termed normal processes. The processes with $n \neq 0$ are termed $U$-processes or Umklapp-processes. The selection rule (5.8) together with the law of the energy conservation is very restrictive. However, for highly excited states, which are almost classical states, there are so many allowed transitions that the selection rule (5.7) is inoperative. This is in agreement with the general rule (cf. for example [15]).

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